BENZENE'S INFERNO, PART II: AUTOMATED ANALYSIS AND IDENTIFICATION

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With the advent of broadband microwave spectroscopy, rotational spectra can now be routinely acquired of many gigahertz of frequency bandwidth. When applied to chemical mixtures of unknown composition, however, spectral analysis often becomes tedious and time consuming. Electrical discharges are examples of complex mixtures with rich rotational spectra, owing to fragmentation of stable molecules and rapid chemical reactions that subsequently take place in the energetic plasma. In this talk, we describe a workflow — which we have developed in Python — for analyzing the products in a benzene discharge. The workflow is designed to be reproducible, automated, and open-source, and can be applied to help assign both laboratory and astronomical spectral line surveys. As part of this workflow, we will discuss how entirely new molecules — those that give rise to strong rotational lines but whose stoichometry and structure are unknown — can be analyzed and identified with minimal chemical intuition.